National Aeronautics and Space Administration

Goddard Earth Science Data Information and Services Center (GES DISC)

ACOS Level 2 Standard Product Data User's Guide, v2.9

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Revision History

Revision Date	Changes	Author
1 October 2010	Initial Release	C. Avis
20 December 2010	Updates to most sections including changes to ACOS metadata/elements based on the v2.8.00 delivery. Updated quality provided by G.Osterman.	E. Martinez
30 October 2011	Complete revision of document. Includes updates for Build 2.9	E. Martinez
29 November 2011	Revb: Updated links to Mirador, corrected typos	E. Martinez
7 December 2011	Revc: corrected typo on page 17 and added additional instructions on how to get data in section 4.	E. Martinez

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1. Introduction

1.1. Scope and Background

This document is intended to provide an overview of the v2.9 Atmospheric CO_2 Observations from Space (ACOS) data product, key features and issues, preliminary validation information, recommendations on data usage, as well as background on the Greenhouse Gases Observing Satellite (GOSAT) mission measurements and the ACOS algorithm. The later sections provide the reader with information on filename conventions and a detailed guide on the format and fields in the hdf product.

This is the third 'public release' of ACOS data, the previous version being v2.8, which was released beginning in February 2011. The v2.8 data are described in a series of validation papers published in 2011. This document updates findings from these papers for v2.9, and gives more general information on the use of ACOS data.

1.2. Overview of Document

The remainder of this section describes the usage of the ACOS data. Section 2 provides details of the differences in this version, product characteristics, validation status, key data fields and ends with recommendations for data analysis. Section 3 provides background information on the GOSAT mission, ACOS file and data conventions, and a complete listing of metadata elements in the v2.9 ACOS data product. Section 4 lists tools to view and search the data products. Section 5 lists contact information for both GOSAT and ACOS data, and the last section lists acknowledgements and relevant publications.

1.3. Data Usage Policy

This data has been produced by the ACOS project, and is provided freely to the public. The ACOS project has been made possible by the generous collaboration with our Japanese colleagues at Japanese Aerospace Agency (JAXA), National Institute for Environmental Studies (NIES), and the Ministry of the Environment (MOE). The L1 data have been made available for this project through an RA agreement between the GOSAT Three Parties and Caltech. To improve our product and have continued support for this work, we need user feedback and also have users acknowledge data usage. Therefore, we request that when publishing, please acknowledge NASA and the ACOS/OCO-2 project.

- Include OCO-2 as a keyword to facilitate subsequent searches of bibliographic databases if it is a significant part of the publication
- Include a bibliographic citation for ACOS/OCO-2 data. The most relevant citations currently are Wunch et al (2011) and O'Dell et al (2011).
- Include the following acknowledgements: "These data were produced by the ACOS/OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the ACOS/OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center."
- Include an acknowledgement to the GOSAT Project for acquiring these spectra.
- We recommend sending courtesy copies of publications to the OCO-2 Project Scientist, Michael.R.Gunson@jpl.nasa.gov.

2. V2.9 ACOS L2 Data Products

2.1. Differences Between v2.8 and v2.9

The following is a summary of the key L1B changes made in v2.9 compared to v2.8. Note that more details of the L1B versions are included in Section 3.2.

- Updated time-varying calibration coefficients received from JAXA in November 2010
- Time dependent correction had been applied only to radiances but not to the noise estimate in v2.8. As a result, fewer and fewer retrievals passed the quality flag over time in version v2.8. In v2.9, the time-dependent calibration correction is applied to both the radiances and the noise estimate, so there is no longer a time dependence in the number of data passing the quality flag.
- Custom glint flag calculation: In v2.8, the JAXA-defined glint flag was used to select data for processing as glint. Due to an error in that flag (that continues to exist in the current data files), this resulted in missing glint data, with more and more data missing over time. We now implement a custom flag for glint, and have full coverage.
- Added L1B noise elements with _l1b suffix
- Added geometric correction factors to L1B geolocation

Changes to the L2 products are as follows:

- Significantly affecting the retrieval results
  - Applied a zero-level offset correction in the A-band to reduce bias in O_2 fits that depends on signal level. By adding a flat zero-level offset term in the state vector and fitting for it, many systematic biases were eliminated. However, this has caused differences between retrievals on M and H-gain data to increase; this issue is being investigated and will be addressed in v2.10.
  - Rescaled O_2 A-band cross sections with a constant factor of 1.025 in order to reduce a surface pressure bias of 10hPa. Mean surface pressure is now unbiased & retrieved aerosols optical depths are somewhat lower; X_{CO2} is in better agreement with ground based Total Column Carbon Observation Network (TCCON) data. The scaling of the O2-A band increased the X_{CO2} values by approximately 4 to 5 ppm.
  - Added ILS interpolation. Previously, the ILS tabulated data were used over fixed wavenumber ranges; they are now interpolated linearly to each target wavenumber. The impact of this change is that X_{CO2} is now 1.5ppm closer to TCCON, and potentially reduced scatter in the retrievals.
  - Glint noise treatment: In v2.8, the ocean scenes were assigned noise values supplied by JAXA, and had very large values of chi-squared, whereas the land scenes had an empirical noise applied, which was more consistent across bands and resulted in chi-squared values close to 1. In v2.9, the empirical noise has been applied to both the ocean and land scenes.
  - Cloud screening applied to glint and land data in preprocessing. In v2.8, it was applied only to the land data in preprocessing.

- Within the code
  - Static input data moved to a single HDF file
  - Upgraded LIDORT version to 3.5T
  - Reworked Jacobian calculations to use automatic derivatives
- Instrument capability
  - Added support for FTS Instrument in up-looking mode
  - Added support for OCO-2 instrument mode
- Speed improvement
  - Use only two streams in the Low Streams Interpolator (LSI) part of the radiative transfer code when a low number of streams is required (was 4 previously).
- Spectroscopy
  - Version 3.3 ABSCO tables were used

2.2. Validation Status

The version 2.9 ACOS X_{CO2} data product has undergone a preliminary validation using roughly 15 months of data, but only H gain over land. Validation against TCCON data shows the v2.9 X_{CO2} has smaller biases at most TCCON stations than v2.8, and significantly reduced scatter as compared to v2.8. In some cases, the scatter has been reduced by as much as a factor of two. The overall bias in the v2.8 data was approximately 7 ppm and much of that has been removed in the v2.9 retrievals (see Figure 1). The mean global bias is now about 0.13 ppm (1.97 ppm standard deviation), though that number does have a small seasonal variation. Figure 2 shows a histogram of the differences between TCCON and ACOS estimations of XCO_2.

A monthly bias number for v2.9 X_{CO2} is shown for several TCCON stations in Table 1. The bias calculation uses only 12 months of data and a full analysis of the bias will be performed upon completion of the v2.9 processing. The numbers in the table are the bias in the monthly mean value of X_{CO2} (TCCON-ACOS). The coincidence criteria is to use ACOS data within 3 hours and 500 km (radius) of the TCCON site and uses only land H-gain data. The seasonal variation in the bias can be seen in the numbers in Table 1 and also in Figure 3, which shows the comparison for the Lamont site (same coincidence criteria as the table).

Overall, the key approach to validating the ACOS X_{CO2} is provided in Wunch et al., (2011). The paper describes a method of evaluating systematic errors in space based column CO_2 measurements. The authors use the uniformity in X_{CO2} poleward of 25° S, to identify a large bias and additional smaller biases due to retrieval or instrument effects in the v2.8 ACOS data. First applying multivariate linear regression analysis to ACOS v2.8 data (after removing the larger bias in the v2.8 X_{CO2}), the authors showed that the remaining bias can be partially removed by applying corrections related to blended albedo (defined in section 2.5.1 below), surface pressure error, airmass and signal in the oxygen band. Definitions of the regression terms are provided in equations 1-4 of Wunch et al., (2011).

A preliminary repeat of the regression analysis for the v2.9 data shows that same four parameters can be used to remove the bias. The regression coefficients change somewhat for v2.9, but those parameters can still be utilized (Wunch et al., 2011). Preliminary analysis using v2.9 data also shows that "blended albedo" can be replaced by using only the oxygen band albedo.

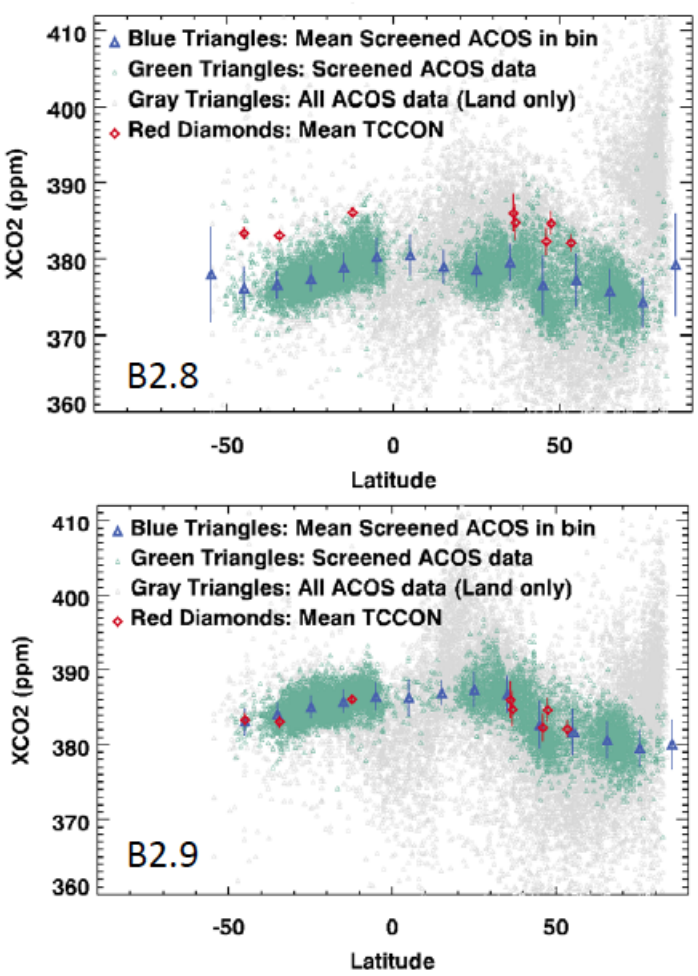

Figure 1. Comparison of ACOS v2.8 (top panel) and v2.9 (bottom panel) XCO2 data compared to TCCON. The consistent (~7 ppm) bias seen in v2.8 has been removed in v2.9.

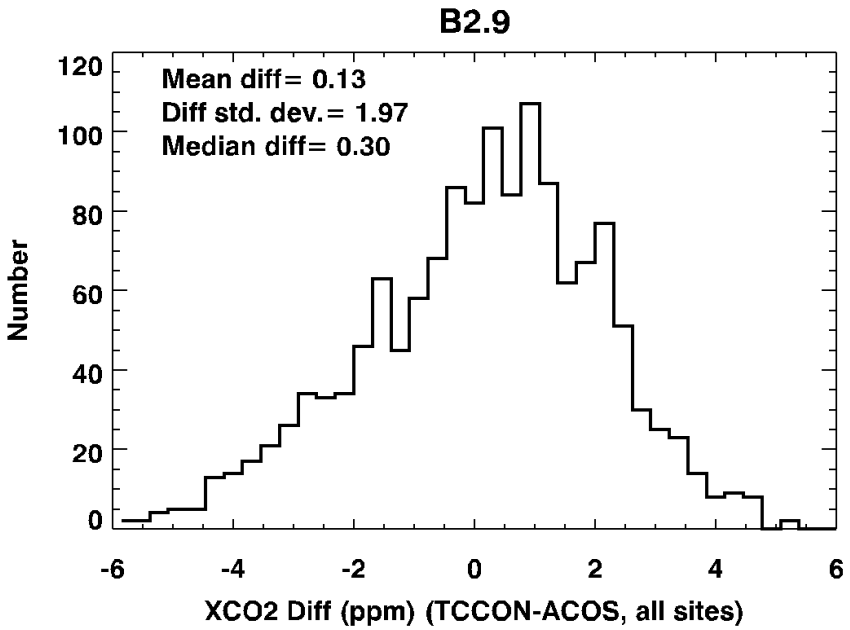

Figure 2. Histogram of the difference between TCCON and ACOS for all TCCON sites used in the analysis.

Table 1. Total mean bias between ACOS v2.9 and TCCON data (Column 2) and monthly mean bias.

Site	Mean Bias	2009 July	2009 Aug	2009 Sep	2009 Oct	2009 Nov	2009 Dec	2010 Jan	2010 Feb	2010 Mar	2010 Apr	2010 May	2010 June	2010 July
Eureka	-1.56													-1.0
Sodankyla	-2.11											-2.1	-2.4	-0.8
Orleans	0.1			0.2	0.2	1.2			3.4	3.0	-0.3		-3.1	-2.0
Garmisch	-0.99		-0.6	0.1	-0.8					1.4	-1.2	-2.4	1.0	-3.1
Park Falls	-0.07	0.8	0.9	0.1	1.0	0.7				1.4	-0.2			
Lamont	0.91	0.6	0.3	-0.2	-0.1	0.8	2.4	2.0	2.2	2.1	1.1	-0.2	1.1	0.2
Tsukuba	-0.94		1.3	-2.0	-1.4	-1.8	-0.4	-1.2	-0.2	-0.6				
Darwin	0.66	0.7	0.6	0.7		1.3								
Wollongong	-0.92	-1.5	-1.7	0.2		-1.5	-2.2			-0.4	-0.7			-0.5
Lauder	-0.59			-1.1					-0.3			-0.2		

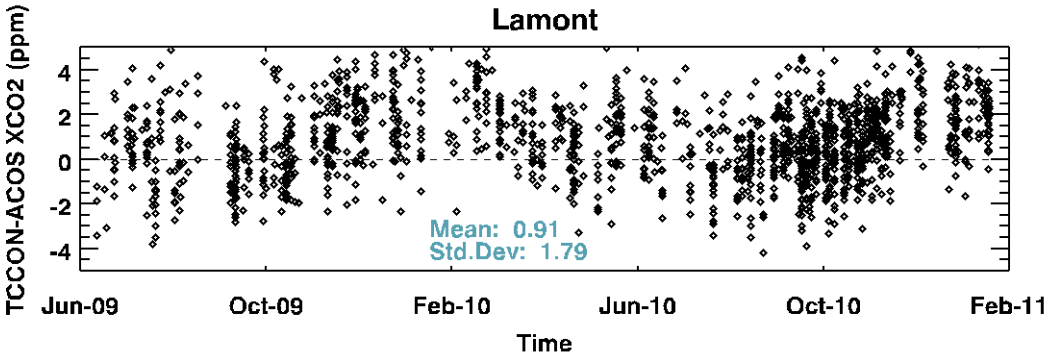

Figure 3. Time series of the bias in ACOS relative to TCCON (TCCON-ACOS) for the TCCON site in Lamont, OK.

2.3. Data Description and User Alerts

The products generated by the ACOS software *build_id* v2.9.00 have the following characteristics that the user should be aware of:

GOSAT data are taken in two gain settings: Medium (M) over bright land surfaces (typically desert regions), and High (H) over all other surfaces. It has been found that while the newly-implemented zero-level-offset (ZLO) fit in the oxygen-A band typically finds positive ZLO for H-gain soundings, a negative ZLO is typically retrieved for M-gain soundings. This negative ZLO drives the retrieved surface pressure negative, such that there is a roughly -5 hPa bias in the retrieved surface pressure for M-gain soundings. This leads directly to a +1.5 ppm average bias in X_{CO2} for M-gain soundings. Users should therefore use caution when attempting to use M-gain data; they may wish to abandon it altogether, or apply their own bias-correction scheme to put it on the same footing as H-gain observations.

Data Completeness/Coverage

- The first two months of GOSAT operations (April and May, 2009) have incomplete operational coverage due to on-orbit calibrations and checkout activities. Full coverage begins about 3 June 2009.
- Level 2 Data using GOSAT L1B version 130130 (April 19, 2011 through present operations) are now retrieved and data products are available. These products have not been evaluated for data quality. When the evaluation is complete information will be provide on the OCO-2 web site and in an updated revision of this document.
- The ACOS Project plans to generate Level 2 products for all available operational GOSAT data (assuming all corresponding ancillary data sets are available).
- Typically data products contain 10-100 useful soundings per orbit, out of the 600-700 L1B soundings collected in an orbit. Note that over 50% of the data is not processed because it does not pass the first cloud screening pre-processing step. A large fraction of data is collected over ocean but not in glint, and thus is not processed. Of the ~100 soundings that are processed for each orbit, convergence and quality screens identify about 20% of that data as good. This is composed of about 15% good soundings over land and 5% over ocean.

- If data users create maps of the filtered v2.9 carbon dioxide data, they should expect to see glint measurements move north and south during the year. Preliminary maps of the v2.9 X_{CO2} retrievals are shown in Figure 4. The monthly mean X_{CO2} maps of the ACOS v2.9 data, include both nadir and glint soundings. Each symbol on the map indicates the average of all X_{CO2} estimates in a 2° x 2° bin for that month that passed all pre- and post-screening filters.

Cloud Screening

- To further reduce the computation time of retrievals containing clouds, the cloud screening algorithm is applied to this version. It performs a fast, Oxygen A-band only clear-sky retrieval for surface pressure, surface albedo, temperature offset and dispersion multiplier. The retrieved surface pressure and albedo information are combined with the X{2} goodness-of-fit statistic and signal-to-noise ratio to determine if a scene is clear(0), cloudy (1), or skipped (2). See Section 6 for a paper on this topic.

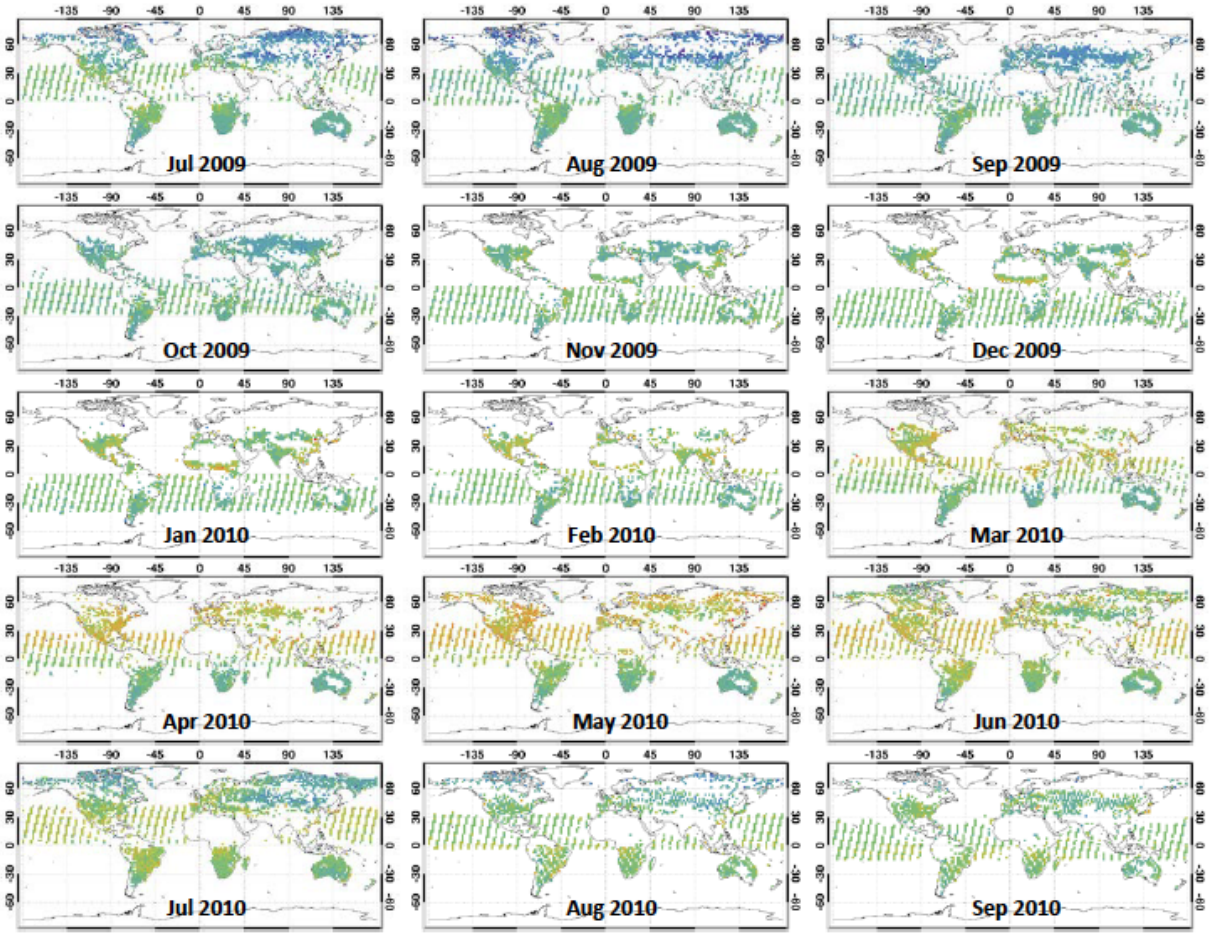

Figure 4. Monthly maps of the ACOS v2.9 X_{CO2} data. Each data point contains the average value for X_{CO2} estimates in a 2° x 2° bin for that month that passed all pre- and post-screening filters.

Post-Processing

- No bias correction – the retrieval results have not been systematically corrected based upon some known reference source
- No post-screening – the results include all soundings whose retrieval converged.
- No post-processing filter has been applied to eliminate soundings based upon certain criteria.

Quality Flagging

- There are several quality flags among the variables. The user should weigh the following information about the flags:
  - *Retrieval_header/sounding_qual_flag* – quality of input data provided to the retrieval processing
  - *Retrieval_results/outcome_flag* – retrieval quality based upon certain internal thresholds (not thoroughly evaluated)
  - *Retrieval_results/master_quality_flag* - four possible values: "Good", "Caution", "Bad", and "Failed" as determined from other flags in the L2 product (see Section 2.3.4)

Averaging Kernels

- The data files include a column averaging kernel value for each retrieved sounding.
- The normalized Averaging Kernel (retrieval_results/xco2_avg_kernel_norm) for a given pressure level is equal to the non-normalized value (retrieval-results/xco2_avg_kernel) divided by the pressure weighting function at that level.

Known Problems

- Content issues
  - The unit listed for *xco2, xco2_apriori, xco2_uncert, co2_profile, co2_profile_apriori, co2_profile_uncert, xco2_uncert_noise, xco2_uncert_noise_smooth and xco2_uncert_noise_interf* is 'VolumeMixingRatio'. The more accurate unit is Mole Fraction with respect to dry air (Mole Mole^{-1}).
- Other
  - Pointers to other files (e.g., 'InputPointer') are not useful because those files reside only on the originating system and were not delivered to the GES DISC
  - The glint flag field does not properly indicate which measurements are taken in glint mode. Use the filter described in Section 2.5.2 instead.

Unassessed Issues

- The L1B versions change over the data record (see section 3.2). We have not performed any significant evaluation of L1B V130130, and we do not have a clear assessment if the resulting L2 products that are consistent with previous L1B version or not. An initial analysis suggests that there are increased differences between land and glint for V130130.

2.4. Key Science Data Fields

2.4.1. Retrieval_results/xco2

The Level 2 Standard Product contains the variable X_{CO2}. This variable expresses the column-averaged CO_2 dry air mole fraction for a sounding. Those soundings that did not converge will not be present. These values are determined by a full-physics retrieval and have units of mol/mol.

2.4.2. Sounding_header/cloud_flag

The Level 2 Standard Product contains the variable *cloud_flag*. This variable expresses the result of an analysis of cloud contamination within a sounding. Every sounding of a granule will have a value: 0 (Clear), 1 (Cloudy) or 2 (Undetermined). The values are determined by an ABO2-band-only retrieval using the FTS spectrum. Only soundings with a value of 0 (Clear) have been processed by the L2 algorithm.

2.4.3. Retrieval_results/surface_pressure_fph

The Level 2 Standard Product contains the variable *surface_pressure_fph*. This variable expresses the retrieved atmospheric pressure at the Earth's surface for a given sounding. Those soundings that did not converge will not be present. These values are determined by a full-physics retrieval and have units of pascals.

2.4.4. Retrieval_results/master_quality_flag

The intention of this flag is to provide general post-processing screening criteria for the Level 2 ACOS X_{CO2} retrievals. The flag provides information for the data user whether a specific retrieval is scientifically usable. However, detailed science analysis using the v2.9 data should utilize a more rigorous data screening formulation that is detailed in the next section. With the master quality flag, there are four possible values: "Good", "Caution", "Bad", and "Failed". The latter case should be rare, but would indicate a problem in the sounding when it was being aggregated into the HDF product.

A "Good" retrieval needs to meet criteria in four areas:

- Cloud screen
- Retrieval success
- Clear sky conditions and surface elevation consideration
- Acceptable algorithm diagnostics

If the retrieval passed the cloud screen and retrieval success tests, but not the final two tests, it is flagged with a "Caution". If the retrieval did not pass the cloud screen and retrieval success tests it is flagged as "Bad".

The master_quality_flag is created from fields in the L2 data product. These fields and the screening criteria are shown in Table 2.

Table 2. Criteria for the L2 master_quality_flag in the v2.9 data

Field Description	HDF Field	Value for Good Retrieval
Sounding_header/Cloud Flag	cloud_flag	0
Retrieval_results/Retrieval Outcome	outcome_flag	= 1 or 2
Spectral_parameters/Chi Squared O2	reduced_chi_squared_o2_fph	< 1.2
Spectral_parameters/Chi Squared Weak	reduced_chi_squared_weak_fph	< 1.6
Spectral_parameters /Chi Squared Strong	reduced_chi_squared_strong_fph	< 1.8
Doubtful Sounding Criteria		
Field Description	**HDF Field**	**Value for Good Retrieval**
Retrieval_results/Total AOD Retrieved	retrieved_aerosol_aod_by_type	< 0.15
Retrieval_results/Surface Pressure Error	surface_pressure_fph – surface_pressure_apriori_fph	-12 – 12 hPa -1200 – 1200 Pa
Retrieval_results/XCO2 a posteriori error	xco2_uncert	< 1.5 ppm
Retrieval_results/Number of diverging steps	diverging_steps	<= 1

2.5. Science Analysis Recommendations

2.5.1. Data Screening beyond the master quality flag

A more rigorous screening criteria, incorporating additional data fields has been developed for use in scientific analysis. This post processing screen can be used for both nadir and glint data. Good soundings will be ones that pass all the criteria in Table 3. The screen has been shown to pass 38% of glint soundings and 14% of nadir soundings for a subset of the data.

Table 3. Advanced screening criteria for the L2 in the v2.9 data

Field Description	HDF Field	Value for Good Retrieval
Sounding_header/Cloud Flag	cloud_flag	0
Retrieval_results/Retrieval Outcome	outcome_flag	= 1 or 2
Spectral_parameters/Chi Squared O2	reduced_chi_squared_o2_fph	< 1.4
Spectral_parameters/Chi Squared Weak	reduced_chi_squared_weak_fph	< 2.0
Spectral_parameters/Chi Squared Strong	reduced_chi_squared_strong_fph	< 2.0
Retrieval_results/Total AOD Retrieved	retrieved_aerosol_aod_by_type	< 0.15
Retrieval_results/Surface Pressure Error	surface_pressure_fph – surface_pressure_apriori_fph	-10 – 10 hPa -1000 – 1000 Pa
Retrieval_results/XCO2 a posteriori error	xco2_uncert	< 1.3 ppm
Retrieval_results/Number of diverging steps	diverging_steps	<= 2
Retrieval_results/Albedo of CO_2 Strong	albedo_strong_co2_fph	> 0.05 *
Blended Albedo	See below	< 1 **
Retrieval_results/Degrees of Freedom	dof_co2_profile	> 1.15 **
* Not used for glint		
** Should not have an effect on glint screening		

The blended albedo screening parameter is a mixture of several albedo terms in the data product files. It can be calculated by using the following relationship:

$$\text{blended albedo} = 2.4A_{O2A} - 1.13A_{SCO2} < 1$$

where A_{O2A} is the albedo for the O2 A band (retrieval_results/albedo_o2_fph) and A_{SCO2} is the albedo in the strong CO_2 band (albedo_strong_co2_fph) as described in Wunch et al. (2011).

2.5.2. Glint Data

Version 2.9 of the ACOS data is the first release that includes glint data that is recommended for use in scientific analysis. While the glint and land data show good general consistency, only very

preliminary analyses have been carried out thus far, so it is impossible to say with certain at what level they agree over all regions of the globe. It appears that the relative difference between nadir and glint soundings degrades after April 19, 2011 (when the L1B data change to V130130).

The glint soundings can be identified using the "retrieval_results/surface_type" field in the Level 2 data files. If this field is "Coxmunk,Lambertian", the sounding is a glint observation. Unfortunately, the field "glint_flag" is carried forward from GOSAT flags, and does not correctly identify data that was processed with the ACOS glint algorithm. The ACOS project evaluates the solar geometry to identify glint and near-glint scenes. Thus, the 'surface_type' is the most accurate way to select glint data.

The actual algorithm used to select data to be processed as glint data is as follows: (a) land fraction is zero, (b) the absolute difference between the solar and sounding zenith angles is less than 2°, and (c) the solar minus the sounding azimuth angles (as defined in the ACOS granules) is between 160° and 200°.

2.5.3. GOSAT H- and M-Gain Data

The TANSO-FTS on the GOSAT satellite makes measurements in different modes. The medium gain (M-gain) is used over very bright surface scenes and is known to have ghosting issues (Suto and Kuze, 2010). These ghosting issues are expected to be corrected in the future, but for now it is recommended that only the "High gain" (H-gain) data from the ACOS data product be used in scientific analyses. The validation analysis by Wunch et al., [2011b] used only H-gain data to determine and correct the bias in the ACOS XCO_2 retrievals.

The gain setting can be determined by looking at the "RetrievalHeader/gain_swir" variable in the ACOS data product. Note that this variable has two character string entries per sounding – one for the S polarization and one for the P polarization.

3. Background Reading

3.1. About the GOSAT Mission

The Japanese GOSAT mission was successfully launched on January 23, 2009. The GOSAT prime mission extends five years from the date it was declared operational on April 19, 2009.

3.1.1. Instrument

The primary GOSAT science instrument is the Thermal And Near infrared Sensor for carbon Observation (TANSO). It is a Fourier-Transform Spectrometer (FTS) with 2-axis scanner. The scanner directs light into two sets of detectors within the instrument.

The Short Wave InfraRed (SWIR) detector is designed to measure the spectrum of reflected sunlight from both land and water surfaces. Three spectral regions are covered in two polarizations:

Band 1	.75 - .78 µm	Oxygen, a.k.a. ABO2
Band 2	1.56 – 1.72 µm	Weak CO_2, a.k.a. WCO2
Band 3	1.92 – 2.08 µm	Strong CO_2, a.k.a. SCO2

The Thermal InfraRed (TIR) detector is designed to measure the spectrum of thermal radiation from both land and water surfaces. A single spectral region is covered (5.5 – 14.3 µm). The ACOS Level 2 products do not include or utilize any TIR data.

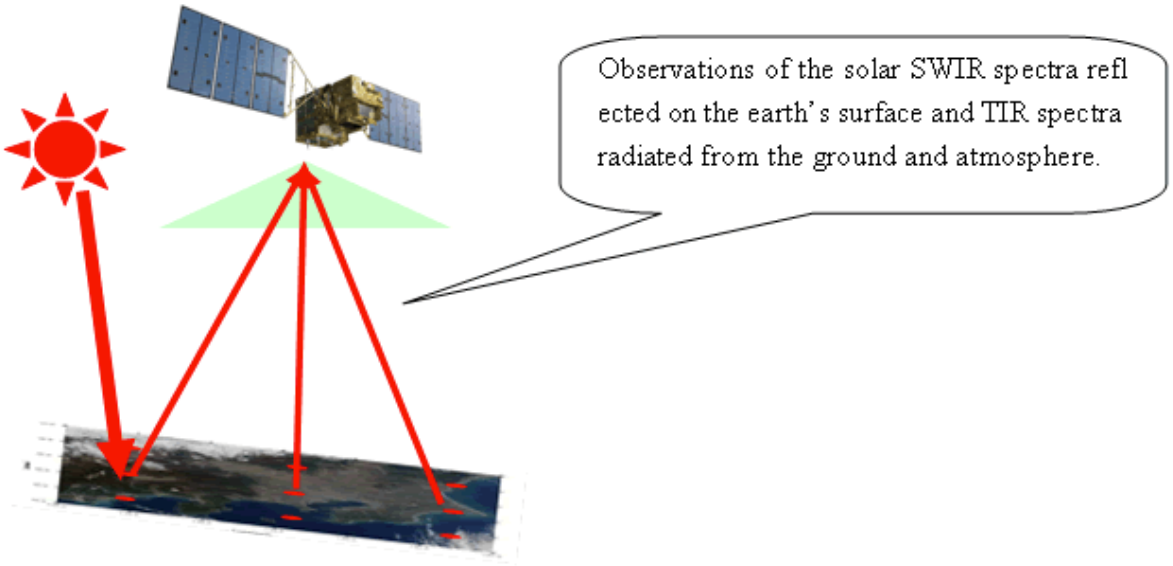

Figure 5. GOSAT Observation Concept

Orbital Parameters

GOSAT nominal orbit parameters are shown below.

- Orbit Type: sun-synchronous, ground track repeat, near-circular orbit
- Recurrent period: 3 days
- Recurrent orbit number: 44
- Revolutions per day: 14+2/3 rev/day
- Local sun time at descending node: 12:45 – 13:15 PM
- Altitude above equator: 665.96 km
- Orbital Period: 98.1 minutes
- Inclination: 98.06 degrees
- Eccentricity: 0.0 (Frozen orbit)
- Longitude at ascending node: Longitude 4.92 degrees west for orbit 1
- Footprint size on ground 10.5 km circle when NADIR viewing

Path ID Definition

The Path ID identifies the GOSAT orbit tracks on the ground. The detailed characteristics are as follows:

- A path begins at ascending node and extends to the next ascending node
- The ascending node of the Path with an ID of 1 is at longitude 4.92 degrees west
- The path number of the orbit tracks westward sequentially
- Path IDs run from 1 through 44
- Path calculator: https://data.gosat.nies.go.jp/map/html_E/MapPathCalendar.html

Note that Figure 6 illustrates 5-point sampling, which was used from April 2009 through July of 2010. Since August of 2010, a 3-point sampling mode has been used.

Points	Interval
1	789 km
3	263km
5 (nominal)	158km
7	113km
9	88km

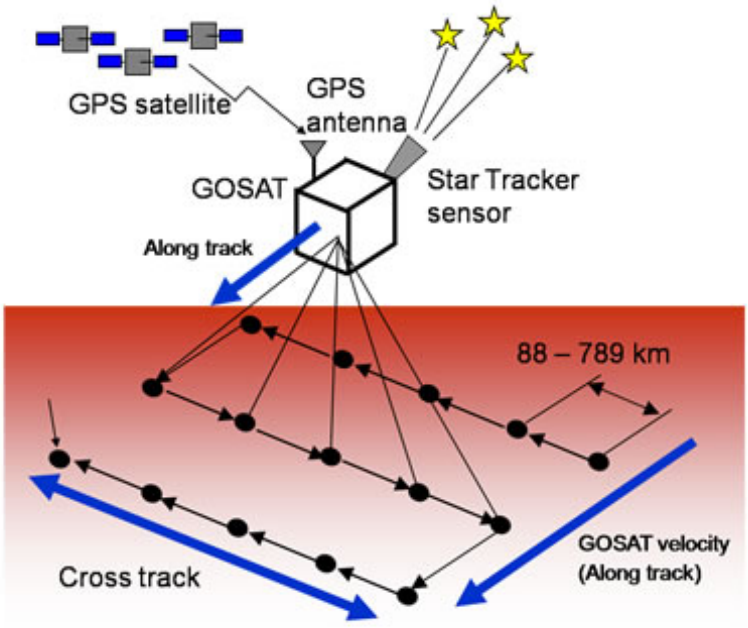

Figure 6. GOSAT TANSO-FTS Observation Details

3.2. GOSAT L1B Releases

The L1B radiance data are provided to the ACOS project by JAXA. As instrument characteristics are better understood, there have been some changes to the L1B data. Table 4 provides a high level view of the L1B versions and key characteristics. Section 3.5.1 shows how the L1B version that was used can be identified in the L2 product file name.

3.3. About the ACOS Task

The ACOS project is part of the Earth System Science Pathfinder (ESSP) Program in the NASA Science Mission Directorate (SMD). The Orbiting Carbon Observatory (OCO) was to have been the first NASA satellite designed to make global measurements of atmospheric carbon dioxide (CO_2) sources and sinks on regional scales at monthly intervals. The failure of the launch system and loss of the observatory therefore represented a setback to NASA's carbon cycle and climate science programs.

To meet its stringent CO_2 measurement accuracy requirements, the OCO Science Team developed and implemented several significant advances in ground-based calibration, validation, and remote sensing retrieval methods. These investments were not lost in the OCO launch failure and remain valuable NASA assets.

The OCO and GOSAT Science Teams formed a close partnership in calibration and validation activities. JAXA granted the ACOS Project access to GOSAT's calibrated Level 1B measurements. The ACOS Project applies the OCO calibration, validation, and remote sensing retrieval assets to analyze these GOSAT measurements. These analyses generate the Level 2 data products described herein.

Table 4. Description of the different GOSAT L1B releases.

Version	Period YYMMDD	Changes
Version006006 (P)	090423–090504 090516–090728	• initial version
Version007007 (P)	090405–090409 090419–090429 090716–091029	• SWIR spectrum unit is changed: (V -> V/cm-1) • SWIR phase correction parameter is changed. (Gauss function parameter; 0.060000 -> 0.002000, see "TANSO Level 1Product Description Document" page 3-29) • Orbital data is changed. (predicted value -> fixed value) • Threshold of sun-glint cone angle is changed. (10 degrees -> 5 degrees) • New product items are added.
Version050050	090405–090409 090419–090503 090602–090731 091028–100208	• TIR phase correction (ZPD shift) • New item on spike noise judgment is added. • Threshold of saturation flag is changed. • Low-frequency correction. flag judgment is improved.
Version080080	090731–091001 100208–100316	• Calibration formula of TIR radiance spectrum are added. (But parameters are modified so that radiance values remain the same as those for V050.) • The accuracy of SWIR spike flag judgment is improved. • "CT_obsPoints" value is changed to "0X0a", when sensor mode is "specific point observation". As a result, it can be distinguished from the case of sensor anomaly. • AT/CT error angles are expressed in GOSAT/TANSO sensor coordinate. • Orbit and attitude parameters are changed.
Version100100	090930–091031 100315–110419	• "The major updated point on Ver.100_100 is that TIR phase correction. There are no change in SWIR processing so there is no difference in SWIR spectrum between current Ver.080_080 and Ver.100_100." - e-mail from Akihiro Matsushima
Version130130	110419–Current	

The GOSAT team at JAXA produces GOSAT TANSO-FTS Level 1B (L1B) data products for internal use and for distribution to collaborative partners, such as ESA and NASA. These calibrated products are augmented by the ACOS Project with additional geolocation information and further corrections. These ACOS Level 1B products (with calibrated radiances and geolocation) are the input to the ACOS Level 2 production process.

The distribution of GOSAT and ACOS L1B products is currently restricted by cooperation agreements between JAXA and NASA.

3.4. ACOS Algorithms

In the sections that follow, the following definitions apply:

- Footprint – an observation by a single instrument
- Sounding – a combined observation of all instruments
- Granule – the construct expressing the content of a product (ACOS product granules contain all the processed GOSAT data for a single orbit)

Level 1B Algorithm Overview

Radiometric calibration (to Level 1B) of the GOSAT TANSO-FTS data is conducted by the GOSAT team prior to delivery to the ACOS team. The GOSAT team utilizes information from calibration observations, such as, internal light sources, deep space observations and lunar observations. These observations are used either directly for Level 1B calibrations or to establish trends for time-dependent corrections.

Further Level 1B radiometric corrections may be applied by the ACOS team using correction tables provided by the GOSAT team.

Sounding and spacecraft geometric variables are included in the ACOS Level 2 products. Some of the derivation ('geolocation') is performed by the ACOS team based upon standard Earth geoid shape and a high-resolution digital elevation model (DEM) and some is copied from the GOSAT input products.

ACOS does not currently process all soundings in an orbit. Because the thermal IR data is not utilized in ACOS, only the soundings in the daylight portion of the GOSAT orbit are processed. This version of processing supports both nadir and glint soundings. Details of glint soundings are provided in section 2.5.2.

In addition, to restrict the attempted retrievals to those with adequate signal, the soundings are also screened by the expression "*sounding_solar_zenith* < 85".

Performing retrievals on scenes containing clouds will either fail or have skewed results (depending upon the extent of cloud coverage). Users should check the *cloud_flag* for the ACOS estimate of scene cloudiness. Many cloudy scenes that are inadvertently passed by the cloud screen algorithm will not converge during the processing and, therefore, will not appear in the Level 2 retrieval results.

Level 2 Algorithm Overview

The Full-physics XCO_2 retrieval algorithm is based on the one that was to be used for the Orbiting Carbon Observatory (OCO). The algorithm is a Rodgers [2000]-type optimal estimation approach and has been described fully in O'Dell *et al*. [2011]. The retrieval algorithm consists of a forward model, an inverse method, and an error analysis step. The overall flow for the retrieval process is shown in Figure 7.

The basic idea is to use a forward model to simulate all three bands of the OCO-2 spectrum then fitting the measured spectra to the model. The forward model contains components simulating the solar spectrum, atmospheric scattering and absorption, surface optical properties, radiative transfer, and detection by the instrument. The input to the forward model consists of meteorological conditions, surface properties, characteristics of the instrument, etc. Everything that is necessary to fully simulate the as-measured radiances must be input to the forward model.

The residuals between the simulated and measured spectra are minimized by changing parameters in the state vector via the inverse method. This inversion is relatively efficient because the forward model returns not just simulated radiances, but also partial derivatives of those radiances, also called Jacobians. The Jacobians are used by the inverse model to efficiently update the state vector in order to quickly find the state that minimizes the residuals.

Once the atmospheric state yielding the best match to the observed spectrum has been found, the algorithm then determines X_{CO2}, errors in X_{CO2} from different sources (such as vertical smoothing, measurement noise, etc.), and the X_{CO2} column averaging kernel. This is necessary because *xco2* is not itself an element of the state vector. Rather, it is determined from the profile of CO_2 , which is part of the state vector. It is formally given by the total number of CO_2 molecules in the column divided by the total number of dry air molecules in the column. This step is labeled "Error Analysis" in Figure 7.

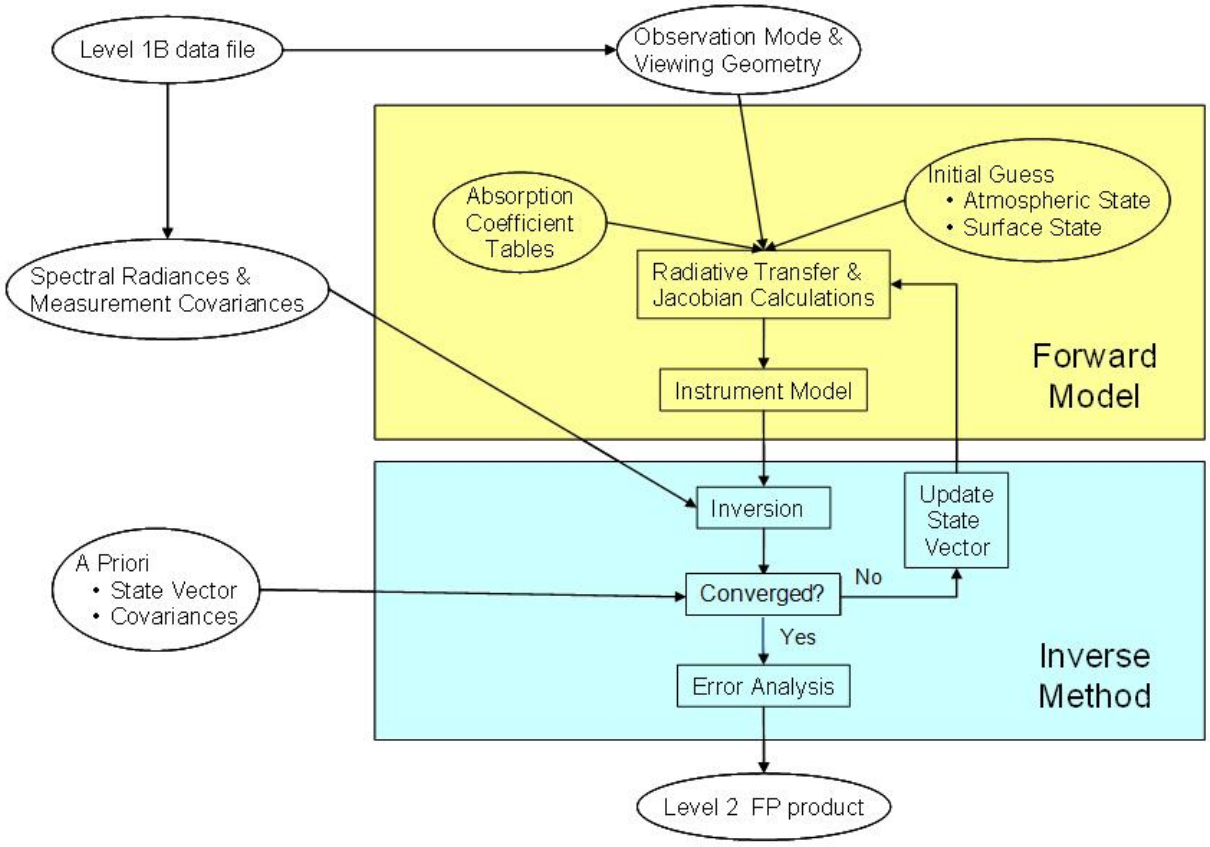

Figure 7. Level 2 Full Physics Retrieval Flow

3.5. ACOS Data Products

The ACOS Level 2 product set consists of products that focus on measuring column-averaged CO_2 dry air mole fraction (*xco2*). The measurements are extracted from observations made by JAXA's Greenhouse gases Observing SATellite (GOSAT). The global coverage that is achieved by GOSAT is repeated every three days at the highest resolution yet achieved from orbit.

3.5.1. File Naming Convention

ACOS Level 2 Product file name specification:

acos_ttt_date_nn_collection_productionTimeStamp**.h5**

Where:

- ttt = product type (L2s)
- date = observation date (yymmdd)
- nn = GOSAT path number (01-44)
- collection label, which consists of the following elements:
  - "Production": indicates a production product

  - v[nnn][mmm]: the TANSO-FTS L1B product version where [nnn] is the algorithm version and [mmm] is the parameter version
  - [software component][version] = the software component and version number that created the product. The software component for the final product is always 'L2s'. The version number for this release is '20900'.
  - r[nn] = the reprocessing level; initial production value is always '01'
  - Pol[x] = the polarization used for the retrievals; possible values are S, P, or B (both)
- productionTimeStamp = production date/time (UTC) at ACOS (yymmddhhmmss)

Filename examples:
acos_L2s_090724_07_Production_v110110_L2s2800_r01_PolB_101204185614.h5

acos_L2s_101102_43_Production_v100100_L2s20900_r01_PolB_111002175250.h5

By policy, *collection* will contain the software *build_id*. In addition, *collection* will also contain a data product version *rNN* in case the same product gets regenerated.

3.5.2. File Format and Structure

All ACOS Level 2 product files are in HDF-5 format, developed at the National Center for Supercomputing Applications http://www.hdfgroup.org/. This format facilitates the creation of logical data structures.

All ACOS Level 2 product files contain data structures indexed by sounding (1 to N soundings/file) and are associated by the *sounding_id* variable in all products.

Variables are combined into groups by type (e.g., SoundingGeometry). Within each type, a variable has one or more values per sounding. Variables may be single-valued (e.g., *sounding_altitude*) or multi-valued (e.g., *co2_profile*).

The metadata of each variable describes the variable's attributes, such as dimensions, data representation and units.

3.5.3. Data Definition

The ACOS Level 2 products contain many variables with a variety of dimensions. The following list describes only the most important of the dimensions.

- Retrieval — the number of retrievals reported (those soundings for which retrievals converged or were converging when the maximum number of iterations was reached)
- Polarization — the number of polarization states
- Level — the number of atmospheric retrieval levels
- Exposure — the number of scans in granule
- Band — the number of spectral bands
- Aerosol — the number of retrieval aerosol types

3.5.4. Global Attributes

In addition to variables and arrays of variables, global metadata is stored in the files. Some metadata are required by standard conventions, some are present to meet data provenance requirements and others as a convenience to users of the ACOS Level 2 Products. The most useful global attributes present in all files are shown in Table 5. Table 6 provides a list of key metadata fields for each variable.

Table 5. Some Global Metadata Attributes

Global Attribute	Type	Description
AscendingNodeCrossingDate	String	The date of the ascending node crossing immediately before the first exposure in the TANSO-FTS file. Format: yyyy-mm-dd
AscendingNodeCrossingTime	String	The time of the ascending node crossing immediately before the first exposure in the TANSO-FTS file. Format: hh:mm:ss.sssZ
StartPathNumber	32-bit integer	The first orbital path on which data contained in the product was collected.
EndPathNumber	32-bit integer	The last orbital path on which data contained in the product was collected.
ProductionDateTime	String	The date and time at which the product was created.
CollectionLabel	String	Label associating files in a collection.
HDFVersionId	String	For example 'HDF5 1.8.5'. A character string that identifies the version of the HDF (Hierarchical Data Format) software that was used to generate this data file.
BuildId	String	The identifier of the build containing the software that created the product.
TFTSVersion	String	The version of the TANSO FTS data used to create this data product.

Table 6. Key Metadata Items

Name	Type	Description
Name	String	The name of the variable
Shape	String	The set of dimensions defining the structure
Type	String	The data representation type
Units	String	The units of the variable.
Minimum	String	Smallest valid value of the variable
Maximum	String	Largest valid value of the variable